

MAR12-2011-006214

Abstract for an Invited Paper
for the MAR12 Meeting of
the American Physical Society

Harvesting the energy from the sun: insights from ab initio materials modeling

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Can quantum and atomistic simulations make valuable contributions to the search of materials for sustainable energy sources? We will address this question by discussing some specific examples where quantum simulations have been used to predict optical properties of nanostructured semiconductors and of complex oxides in contact with water. We will also discuss issues related to the comparisons with increasingly complex experiment.